2-Methoxyethyl acetoacetate

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Model Performance

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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -15.2 °C

Global applicability domain: Inside

Local applicability domain index: 6.97e-01

Confidence level: 5.58e-01

Nearest Neighbors from the Training Set

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Diethyl maleate Measured: -3.65 Predicted: 1.33

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Diethyl (2E)-but-2-enedioate

Measured: -3.65 Predicted: 1.33

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2-Propene-1,1-diol diacetate

Measured: -37.6 **Predicted:** -3.57

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Diethyl propanedioate Measured: -50.0 Predicted: -34.4

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Dimethyl glutarate Measured: -42.5 Predicted: -25.9

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Butanedioic acid, methylene-,

diethyl ester Measured: 58.5 Predicted: 14.9